Neutron Generator Power Supply Modeling in EMMA (U)

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Sandia National Laboratories has prime responsibility for neutron generator design and manufacturing, and is committed to developing predictive tools for modeling neutron generator performance. An important aspect of understanding component performance is explosively driven ferroelectric power supply modeling. EMMA (ElectroMechanical Modeling in ALEGRA) is a three dimensional compile time version of Sandia's ALEGRA code. The code is built on top of the general ALEGRA framework for parallel shock-physics computations but also includes additional capability for modeling the electric potential field in dielectrics. The overall package includes shock propagation due to explosive detonation, depoling of ferroelectric ceramics, electric field calculation and coupling with a general lumped element circuit equation system. The AZTEC parallel iterative solver is used to solve for the electric potential. The DASPK differ-entail algebraic equation package is used to solve the circuit equation system. Sample calculations are described. (U)

Introduction

Sandia National Laboratories has prime responsibility for neutron generator design and manufacturing. EMMA (ElectroMechanical Modeling in ALEGRA) is a three-dimensional compile time version of Sandia's ALEGRA code which is intended to provide a framework for high fidelity modeling of all the major aspects of explosively driven ferroelectric neutron generator function except for the actual particle physics. The EMMA code is built on top of the general ALEGRA (Arbitrary Lagrangian-Eulerian for General Research Applications) code framework for parallel physics computations (Budge and Peery, 1993). The code does solid dynamics calculations and in addition has the capability for modeling the electric fields in dielectrics and associated charge arising in the attached conductors. The overall modeling requirements include shock propagation due to explosive detonation, depoling of ferroelectric ceramics, electric field calculation and coupling with a general lumped element circuit equation system.

This paper provides a status report on the EMMA project and gives a realistic assessment of the progress being made in developing a production predictive capability running on large massively parallel machines. The desire to achieve highly accurate solutions of coupled electromechanical response is a primary driver for the development of this technology on large parallel machines. The general approach for developing a well-integrated software technology is described and several calculations are discussed.

EMMA - Basic Theory

EMMA brings together mechanical modeling based on standard equations of mass and momentum conservation and a general quasistatic electric field solution (Montgomery and Chavez, 1986). The equations are coupled only through material constitutive equations in which the stress is affected by the electric field and vice versa. The theory assumes that the electric field can be well represented by the gradient of a potential. This assumption is valid as long as the time scales of interest are much longer than electromagnetic wave time scales, and currents are small enough to neglect electric field components due to the time rate of change of the magnetic vector potential. Thus materials are broken into two types: perfect conductors and dielectrics. Perfect conductors are indicated by surfaces of constant electric potential. Dielectrics will in general have properties which vary anisotropically in space and time in response to mechanical motion and electric fields. The basic electric field equation to be solved is

$$\nabla \cdot (e \cdot \nabla j) = \nabla \cdot P \qquad (1)$$

where j is the electric potential, P is obtained from the electric displacement, D, by

$$P = D - e \cdot E \,, \qquad (2)$$

where e is the dielectric tensor, and the electric field, E, is obtained from

$$E = -\nabla j \ . \qquad (4)$$

It is assumed that the physical configuration of interest can be modeled by N conducting electrode surfaces which may or may not be connected by conducting elements to the other surfaces and external circuit nodes or elements. These N surfaces form a capacitor system at which charge appears or is discharged. Since the field equations are linear we can write the solution as a linear combination of N fundamental solutions and a particular solution.

$$j = j_p + \sum_{i=1}^{N} V_i j_i \qquad (5)$$

Using the integral form of Gauss's law to calculate the charge on all N conducting surfaces allows derivation of equations relating the charges, voltages, capacitance matrix and source for the system under consideration. In particular, a three-dimensional finite electromechanics code called SUBWAY was developed at Sandia to solve such problems. While this code has been applied to problems of interest, it lacks many features found in ALEGRA and has not been ported to massively parallel machines (Montgomery and Chavez, 1986, Montgomery, et al., 1996).

EMMA Software Components

The EMMA software components include the basic ALEGRA framework for parallel physics calculations, the EMMA field equation generator, the piezoelectric and ferroelectric material model packages, the AZTEC sparse matrix parallel iterative solver package and the circuit equation solver using DASPK for solving the associated differential algebraic equations.

ALEGRA Framework

ALEGRA is a general code platform upon which various physics applications can be built. This platform is written in an object-oriented manner in C++ and is used to assist programmers in building various physics applications. The principal C++ class derivation diagram for EMMA is shown in Figure 1. Qsem is the class name that stands for QuasiStatic ElectroMechanics. The Qse class is concerned only with electric field and circuit equation calculations independent of kinematics and mechanics. The ALEGRA virtual class structure is an extremely convenient and elegant tool for building code to model coupled physics.

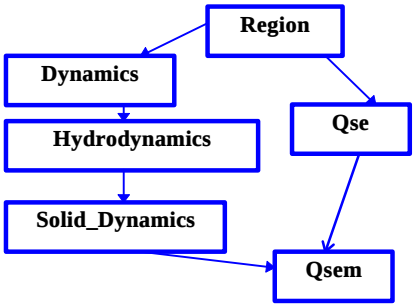

Figure 1. C++ Class derivation hierarchy for EMMA physics modeling.

EMMA Field Matrix Formation

The matrix entries for the potentials centered on the finite elements nodes are derived from numerical integration of the finite element basis functions over the elemental volumes. The contribution of each element to a given matrix entry is

$$a_{ij}^{e} = \int_{V_e} \nabla N_i \cdot \left(e \cdot \nabla N_j \right) dV \qquad (6)$$

and the polarization contribution to the right hand side of the linear system from each element is given by

$$f_i^{\,e} = \int_{V_e} \nabla N_i \cdot P dV \qquad (7)$$

The integrals are evaluated by Gaussian quadrature using the fundamental coordinates of the elements as the independent integration variables. This requires an appropriate transformation of gradients and volume differential at each Gauss point.

AZTEC Solver

AZTEC is a parallel interative solver package written in C which has been developed and is currently supported at Sandia (Hutchinson, et. al., 1995; Shadid and Tuminaro, 1994). AZTEC provides a simple interface for large sparse linear systems on parallel machines. The AZTEC package requires that the user provide connectivity and matrix entry information for the unknowns stored on each processor of the parallel machine, and the package determines all required communications to perform the iterations in parallel. This transformation is performed once each time step. The actual linear solve is performed $N + 1$ times at each time step with different right hand sides. The preconditioned conjugate gradient method is the

method of choice for our problems since the matrix is symmetric. The boundary conditions are applied by setting diagonal elements and right hand sides for the boundary nodes to appropriate large values. This maintains symmetry of the matrix. The initial guess is zero for the initialization step and the last computed solution is used as the initial guess for all subsequent calls to the solver.

We have found that the conjugate gradient iterative solver is generally quite effective. More iterations are required as the number of elements in the mesh increases. The degree of finite element distortion can be checked by examining the determinant of the element deformation gradient at each Gauss point. When this determinant changes sign the code warns of the situation as both the hydrodynamic time step and the conjugate gradient iterative solve will be adversely affected. It is expected that use of EMMA in the future will require both robust Lagrangian numerics and the use of single and multiple material ALE technology.

Piezoelectric and Ferroelectric Material Models

The primary coding taken directly from the previous SUBWAY technology was some FORTRAN 77 material model coding. These models were implemented in EMMA underneath a MIG interface (Brannon and Wong, 1996a,1996b). The MIG interface is a Sandia interface for standardizing the sharing of material model coding. The models installed in EMMA include a linear piezoelectric model, a ferroelectric-antiferroelectric phase transforming model and nonlinear ferroceramic model.

Linear piezoelectric materials can be modeled by the standard equations for stress, T, and electric field

$$\begin{aligned} T &= c \cdot S - e \cdot E \\ D &= e \cdot S + e \cdot E \end{aligned} \tag{8}$$

where S is the strain, c is the elastic stiffness matrix, e is the piezoelectric constant matrix, and e dielectric tensor. The relation for electric displacement gives

$$P = e \cdot S \tag{9}$$

Ferroelectric ceramic materials have a more complicated mechanical and dielectric response. Stress relaxation due to mobile ferroelectric domain movement and phase transformation complicate the constitutive representation. The models currently implemented in code represent the electric displacement by

$$D = P(S,a) + e(S,a) \cdot E \tag{10}$$

where a represents a vector of internal state variables defining the state of spontaneous polarization, phase, and domain alignment of the material which are specified by an additional set of evolution equations.

A major thrust for the coming years will be to test and improve these models to such a point that analysis can be fully predictive. This of course entails a series of experiments to obtain good material constants for use in the models.

Circuit Equation Solver and DASPK

EMMA includes a run-time circuit equation package which allows a fairly general implementation of an arbitrary lumped element circuit which is solved in conjunction with the field equations. Each conductor defined in the mesh is considered as a node in an electrical network. Circuit elements such as resistors, inductors and capacitors can also be defined between these nodes. Circuit element relations provide rules giving the current through the element due to the voltage at the nodes. Conservation of charge is imposed at the circuit nodes. At regular junction nodes the sum of the currents is required to be zero. At least one node in the circuit must have a specified voltage value in order to make the solution unique. This value is usually specified as zero, i.e. a ground. The conservation of charge relation at a ground node is used to indicate the current to ground and corresponds to the ground current diagnostic from a test fixture. The resulting set of equations is a system of differential-algebraic equations (DAE) which can be nonlinear. In general one cannot transform DAE systems into systems of ordinary differential equations (ODEs). Fortunately, these DAE systems have been studied in depth and packages such as DASPK have been developed (Brown, et al., 1994,1995) at LLNL. The FORTRAN 77 DASPK package was obtained, integrated into our code and used very successfully. For limited circuit cases a modified ODE solver taken from the SUBWAY code may also be accessed.

EMMA Calculations

A primary purpose for building the EMMA code was to allow for very large three-dimensional simulations on parallel computers. The intent is to provide enough spatial resolution in the modeling that all experimental features can be captured accurately. Two applications will be described below.

Quartz Gauge

The physics involved in the simulation of a quartz impact gauge are similar to the physics of an explosively driven neutron generator power supply, and it is a problem that has been accurately characterized experimentally (Montgomery, et al., 1996). The

geometry of a fully electroded configuration is shown in Figure 2.

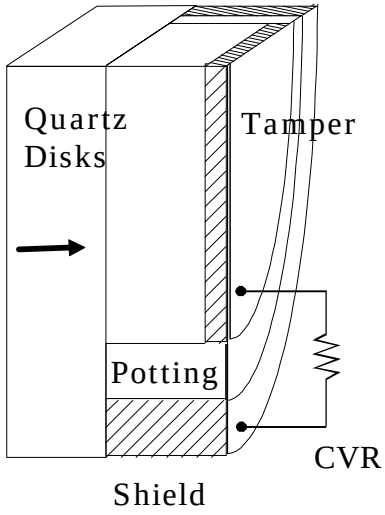

Figure 2. Fully electroded quartz gauge configuration (one quarter of the gauge is shown).

The gauge consists of a disk of X-cut quartz, embedded in an epoxy filler, surrounded by an aluminum shield can and an aluminum tamper. The shield is electrically connected to the impact surface of the disk by means of a thin conducting layer deposited on the surface. As a result of the piezoelectric effect, impact loading of the disk causes a current pulse to flow between the aluminum tamper and shield can, through the low-impedance current-viewing resistor (CVR), as shown. The diameter of the disk is typically much larger than the thickness, so that the stress and resultant electric field are nearly one-dimensional. In order to simplify the mechanical boundary conditions at the impact surface, the impactor is often made of quartz.

Figure 3 shows the results of several simulations, at different resolutions, compared with experimental data. Because quartz is anisotropic, the problem is not axisymmetric (and therefore two-dimensional); however, it is only necessary to model one quarter of the gauge with the appropriate mechanical and electrical boundary conditions at the symmetry planes. Curves are shown for 25 unknowns in the axial direction (3465 elements), 50 unknowns in the axial direction (6615 total elements) and 100 unknowns in the axial direction (52920 total elements).

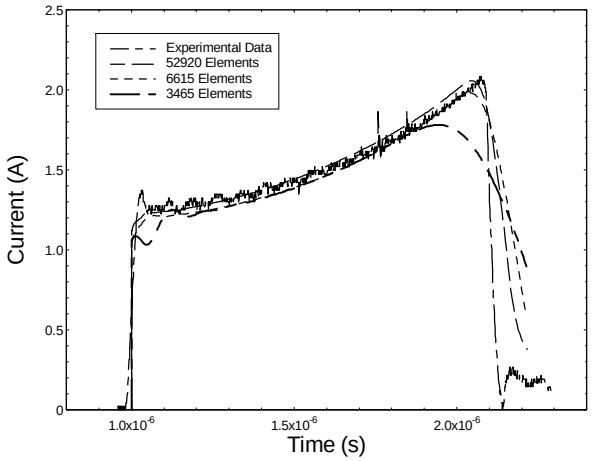

Figure 3. Measured and predicted gauge currents for the fully electroded configuration of Figure 3 (disk thickness = 0.25 in, disk diameter = 0.625 in, alumina-loaded epoxy, radial thickness of the epoxy = 0.125 in, initial impactor velocity = 132 m/s).

The fidelity of the simulation improves significantly as a result of increasing the resolution of the simulation primarily by sharpening the peak and width of the final current pulse shape. These calculations utilized a special nonlinear piezoelectric material model.

Power Supply Calculations

We have run several calculations on the Intel Paragon at Sandia to model a generic power supply gas gun test. A power supply configuration consisting of two rectangular blocks of ferroelectric ceramic embedded in a cylinder of alumina-loaded epoxy was tested. A thin aluminum plate was attached to the end of the cylinder and impacted by a projectile. The alumina-loaded epoxy cylinder had a conductive flame spray on its outside surface to maintain a ground plane and voltages and currents from the power supply were monitored using capacitive dividers and current viewing transformers. As the shock wave generated by the projectile impact propagates through the ferroelectric ceramics the material undergoes a compression driven transformation from the ferroelectric to the antiferroelectric phase. Charge bound to electrodes on the bars is liberated and produces voltage across the ceramic elements. The elements are electrically connected in series with a nonlinear resistive load which maintains the voltage at a relatively constant level once the capacitive charge on the active ceramic elements has reached the regulation voltage.

In the calculations described below we used a pressure boundary condition instead of an impactor to generate a shock wave. As the shock wave propagates

through the bars, the fe-afe phase transforming ceramic material model modifies the material polarization as well as the dielectric tensor and the circuit begins to respond. The idealized nonlinear resistor circuit element permits only very small amounts of current to pass through until the required regulator voltage is reached. The current and total charge traces in Figure 4 show the initial depoling of the ceramic and charge build up as evidenced by the current to ground traces from the conducting shell or can (can current). After the required voltage is reached the current flows from the stack to ground (stack current) through the regulator element. The total can charge trace is lower in value and of shorter duration than the experimental data due to a difference in the length of the ferroceramic bars. The capacitances are also biased from features not modeled in this calculation. The computed current traces are noisy due to uncorrected problems with the ferroceramic model we have been using. The power supply current is the current off the base of the stack to ground which should balance the sum of the can and stack currents.

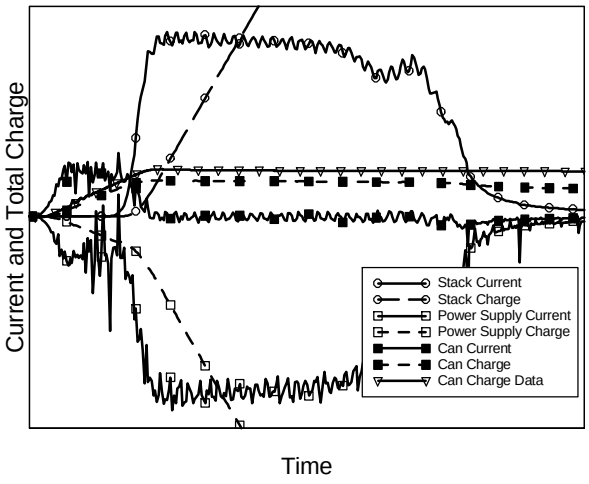

Figure 4. EMMA simulation of gas gun experiment. Charge is the time integral of current.

Conclusions and Future Work

Experience to date indicates that the EMMA architecture provides an excellent framework for production simulations of defense program components requiring electromechanical modeling. The code will clearly help delineate the difficult issues associated with dielectric material properties and interactions with the details of the shock propagation through ferroelectric materials. The basic groundwork for this modeling effort appears to be solid. Areas needing improvement include robust scalable mesh generation and parallel decomposition, material modeling, turn around time for calculations and robust postprocessing capability for large problems. A program is in place to improve and validate the material modeling through both theoretical and experimental components. The new ASCI computing machines should provide the computational power to make highly resolved calculations fairly routine as the issues of robust scalable mesh generation and postprocessing are resolved.

Acknowledgment

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